DMRG study of the spin gap in a one dimensional Hubbard model: effect of the distant transfer and exchange coupling

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Abstract

The spin gap of a one-dimensional repulsive Hubbard model is numerically calculated with the density matrix renormalization group, with a special emphasis on the effect of a next-nearest neighbor hopping (t') and the nearest-neighbor ferromagnetic exchange (J) interaction. At half-filling, a significant spin gap opens if $|t'| \simeq |t|$ and $J = 0$, in agreement with the weak coupling theory, while the gap is strongly suppressed by the introduction of J. On the other hand, the quarter-filled system has very small spin gaps regardless of the values of t' and J. Implications for the CuO_2 chain in $Sr_{14}Cu_{24}O_{41}$ and related materials are discussed.

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For the past several years, the spin gap in strongly correlated one dimensional systems has been a focus of attention. Intensive studies have been done on ladders[1-7] and systems with dimerized[8] or frustrated[9] spin-spin interactions. Interests arose, since some of these studies have revealed that the existence of a spin gap can lead to a dominance of pairing correlations even in purely repulsive models.

More recently, one of the present authors studied a one dimensional (1D) Hubbard model (t-t'-U model) that contains next-nearest neighbor (NNN) hoppings in addition to nearest-neighbor (NN) ones. Making use of a weak-coupling renormalization, he has predicted the existence of a spin gap in a certain parameter regime.[10] A notable observation there is a prediction of a *superconductor-insulator* transition occurring at some finite Hubbard interaction $U = U_C$ at half-filling, for which three of the present authors subsequently have identified such a transition at a finite U with quantum Monte Carlo (QMC) and density matrix renormalization (DMRG) methods.[11]

The 1D t-t'-U model is thus theoretically interesting, where the system has both a frustration (arising from the interference between t and t') and a character of a ladder as mentioned below. The model with $|t| \sim |t'|$ (where interesting physics is expected) may also have some relevance to real materials such as the cuprates that contain 1D chains. Specifically, a recently discovered superconductor, $Sr_{14-x}Ca_xCu_{24}O_{41+\delta}$[12], and related materials possess layers consisting of 1D chains alternating with layers of two-leg ladders. In the chain, the NN (Cu-Cu) transfer (t) should be reduced due to the 90° Cu-O-Cu bond angle, just as in the inter-ladder hopping (estimated to be ~ 0.1 eV[13]) in the ladder layers. The NNN transfer (t') in the chain is in turn equivalent to the NNN transfer (estimated to be ~ 0.1 eV[14]) in the CuO_2 plane in the 2D cuprates. We then end up with $|t| \sim |t'|$ for the chain. In fact, recent band calculation for $Sr_{14}Cu_{24}O_{41}$ shows that $t = -0.09$ eV and $t' = -0.17$ eV.[15]

To be more precise, the effect of small t not only gives rise to a large ratio of $|t'/t|$, but also results in a net ferromagnetic NN exchange in real materials. Namely, the real materials has a ferromagnetic exchange interaction between NN Cu sites due to the exchange between Cu3d and O2p orbitals[16,17] and the Hund's coupling between the Op_x and Op_y orbitals.[13]

Since the antiferromagnetic NN interaction ($\sim 4t^2/U$) is small, the net NN interaction turns out to be ferromagnetic with an order of few hundred K in $La_6Ca_8Cu_{24}O_{41}$.[17] Such an ferromagnetic interaction is not included in the t-t'-U model since the oxygen orbitals are not explicitly considered. In order to take this effect into account, we should add a NN ferromagnetic exchange J to the t-t'-U model to have the 't-t'-U-J' model.

In $Sr_{14}Cu_{24}O_{41}$, for which the experiments suggest that the average Cu valence in 1D chains is around $+2.5$, a spin gap of about 140K is observed.[18−21] The origin of the spin gap is yet to be established theoretically. On the other hand, in $La_6Ca_8Cu_{24}O_{41}$, where the average Cu valence is $+2$, such a spin gap is not observed in the 1D chain, and the system behaves as nearly free spins. Since the weak-coupling theory predicts the existence of the spin gap in the t-t'-U model in a certain parameter regime, it would be intriguing to see if the experimental observations can be explained by the effect of the sizeable $|t'/t|$. In $La_6Ca_8Cu_{24}O_{41}$, to be more precise, the magnetic susceptibility can be fitted with the Curie-Weiss law with a Curie temperature of $\sim 10K$[18,20], which is much smaller than the NN ferromagnetic exchange mentioned above. It would also be interesting to investigate whether such an observation can be understood within the interplay of t' and J.

The purpose of the present paper is to evaluate the spin gap in the t-t'-U and t-t'-U-J models using DMRG, and to compare the results with the experimental observations for the cuprates. Since the Cu valence $+2$ and $+2.5$ corresponds to the band filling $n = 1$ (half-filling) and $n = 0.5$ (quarter-filling), respectively, we focus on these fillings.

Let us start with the t-t'-U model. The Hamiltonian is given, in standard notations, as

$$\mathcal{H} = -t \sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) - t' \sum_{i\sigma}(c_{i\sigma}^\dagger c_{i+2\sigma} + \text{h.c.})$$
$$+U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where t, (t') are NN (NNN) hoppings and U is the Hubbard repulsion. The sign of t does not change the physics because it can be changed by a gauge transformation. Thus, we take $t > 0$ without a loss of generality. On the other hand, the sign of t' is crucial when the system deviates from half-filling, at least in the weak-coupling theory. Here we take $t' < 0$

in accord with the cuprates.

Let us first recapitulate the weak-coupling result.[10] When the system is mapped to the Tomonaga-Luttinger (TL) model, the system with a small enough $|t'/t|$ reduces to the $t' = 0$ case, since they are essentially the same in the vicinity of the Fermi level. For a substantial $|t'|$, on the other hand, the Fermi level intersects the one-electron band at four k-points ($\pm k_F^1$ and $\pm k_F^2$). Namely, there are two right-moving and two left-moving branches in the terminology of the TL model. When the Umklapp processes are absent, the situation is, as far as the weak-coupling picture is concerned, essentially identical to the two-leg Hubbard ladder, where a spin gap opens when the two Fermi velocities are not too different.[4] Thus, a spin gap opens in the present model as well for a certain range of the ratio of the Fermi velocities, i.e., for $|t'| > t_c'(n)$.

Bearing this in mind, let us now turn to the numerical calculation of the spin gap performed by DMRG. We take several typical values, namely, $t' = -0.55, -0.8$, and -2.0 (hereafter $t = 1$ is taken as a unit of the energy). As for the value of U, we take $U = 8$ for $t' = -0.55$ and $t' = -0.8$, and $U = 16$ for $t' = -2$. We have taken such large values of U because otherwise the spin gap strongly fluctuates with the number of sites. The fluctuation becomes worse for large $|t'|$, so that we take $U = 16$ for $t' = -2$. Fortunately, large U is of physical interest, since we can probe the strongly correlated systems such as the cuprates.

Generally, the spin gap is much smaller than the charge gap, so an accurate calculation is required. The calculation has been done for system sizes up to $L = 56$ sites for $t' = -2$, and $L = 48$ sites for $t' = -0.55$ or -0.8. We kept up to 300 states per block, and stored the transformation matrix to construct the initial state for each superblock diagonalization.[22] After each diagonalization, the accuracy of wave function is improved by the inverse iteration and conjugate-gradient optimization, where the truncation error is $\sim O(10^{-5})$.

The spin gap of a system with N up-spin and N down-spin electrons is calculated by the equation,

$$\Delta_S = E(N + 1, N - 1) - E(N, N),$$

where $E(N_\uparrow, N_\downarrow)$ is the ground state energy of a system with $N_\uparrow$ up spin and $N_\downarrow$ down spin electrons.

We first look at the spin gap for $t' = -0.8$ with $U = 8$ in Fig. 1, which plots Δ_S against the inverse of the system size, $1/L$. By least-square fitting the result with second order polynomials in $(1/L)$, we evaluate the spin gap in the thermodynamic limit. For half filling it is estimated to be $\Delta_S = 0.16$. At quarter filling, the spin gap becomes very small, but is still finite as far as the present fitting is concerned. For $t' = -0.8$, the Fermi level intersects the one-electron band (which has double minima) at four k-points both for $n = 1$ and $n = 0.5$, where the two Fermi velocities have comparable magnitudes. Hence our result is consistent with the weak-coupling theory, which is nontrivial since U here is quite large.

Next we turn to the spin gap for a smaller $t' = -0.55$. For this value of t', the Fermi level at half-filling still intersects the one-electron band at four points, but the inner pair is close to the local maximum ($k = 0$), where the Fermi velocity is very small. According to the weak-coupling theory, the spin gap does not open if the ratio of the two Fermi velocities is too small (or large). Our DMRG result for $U = 8$ in Fig.2 indeed shows that the spin gap closes or becomes negligibly small.

At quarter-filling the system with $t' = -0.55$ and $U = 8$ turns out to be *ferromagnetic*, as confirmed by DMRG calculation of the total energy and the total spin. This is in accord with previous studies[23−25] showing that the ground state of the t-t'-U model is fully spin-polarized for sufficiently large U, small (but finite) t', and fillings away from half-filling.

Finally, we show the spin gap for a larger $t' = -2$ with $U = 16$ in Fig. 3. To further reduce the finite size effect, we choose the system size of $4\times$ integer electrons. At half-filling, the spin gap in the present fitting opens in agreement with the weak-coupling theory, but it is much smaller than that for $t' = -0.8$. For the half-filling, a comparison with a DMRG result for the J-J' Heisenberg model (Heisenberg model with NNN antiferromagnetic exchange) by White and Affleck[26] may be interesting. According to their result, the magnitude of the spin gap as a function of J'/J takes its maximum at $J'/J \simeq 0.6$, and becomes much smaller for $J'/J > 2$. If we assume $J = 4t^2/U$ and $J' = 4t'^2/U$, we can then draw a consistent picture

that the magnitude of the spin gap of the t-t'-U model takes its maximum at $t' \simeq -0.8$, and is very small for $|t'| > \sqrt{2}t$.

At quarter-filling for $t' = -2$, the magnitude of the spin gap further decreases to become negligibly small in the thermodynamic limit (unless the curve upturns around $1/L \sim 0$). If the spin gap does exactly vanish, this cannot be understood within the weak-coupling theory because the Fermi level intersects the band at four points, and the ratio of the Fermi velocities is not large. The intraband umklapp processes are known to suppress the spin gap in the Hubbard ladders,[4–6] but for $t' = -2$ and $n = 0.5$ in the present model, processes corresponding to the intraband umklapp do not exist. Then, the disappearance of the spin gap in the region of large U, if any, would be beyond the scope of the weak-coupling theory.

To summarize the above results, a relatively large spin gap opens at half-filling for $|t'| \simeq t$, while at quarter filling, either the magnitude of the spin gap becomes smaller, or the ground state becomes ferromagnetic. The suppression of the spin gap for $n = 0.5$ may be reminiscent of the results of the t-J-J' model obtained by Ogata et al, where the spin gap at half-filling is destroyed by hole doping.[9] We stress that this is not trivial since the effective Hamiltonian of the doped t-t'-U model in the large U limit is not the t-J-J', but the t-t'-J-J' model, where the NNN hopping may play an crucial role.

We move on to the result for the t-t'-U-J model with the Hamiltonian

$$\mathcal{H} = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) - t' \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+2\sigma} + \text{h.c.})$$
$$+ U \sum_i n_{i\uparrow} n_{i\downarrow} - J \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{4} n_i n_j \right),$$

where $J > 0$ is the ferromagnetic exchange. In Fig. 4(a), we show the result for the spin gap when $J = 0.5$ or 1.0 is present for $t' = -0.8$, $U = 8$ at half-filling to compare with the result for $J = 0$. We can see that the even the spin gap for $t' = -0.8$, which has a relatively large value in the absence of J, is almost completely suppressed by $J = 0.5$. Intuitively this is because the spin-gap behavior arising from the effect of t' is 'canceled out' with the effect of J, which suppresses the spin fluctuations. Since the spin gap takes its maximum around $t' = -0.8$ for $J = 0$, the present result suggests that $J = 0.5$ is enough to suppress the spin

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gap at other values of t'. At quarter filling, where the spin gap is extremely small already at $J = 0$, the introduction of J further destroys the gap as shown in Fig.4(b) for the case of $J = 0.5$ or 1.0 with $t' = -2$, $U = 16$.

In both the half- and quarter-filled cases, large enough J should produce a ferromagnetic ground state. For the present values of J and the system sizes, we do not have a ferromagnetic ground state, as seen from the fact that the spin gap (at each system size) is finite. However, we do have a possibility that a ferromagnetic ground state is realized in the thermodynamic limit, especially in the cases where the extrapolated spin gap is negative, as in $n = 1$ and $J = 1$, or in all quarter filled cases.

Let us finally comment on the implications of the present results on the experimental observations. In $La_6Ca_8Cu_{24}O_{41}$, the magnetic susceptibility in the 1D chains does not indicate a spin gap. Our numerical results suggest that this can be explained within the half-filled t-t'-U-J model. Namely, the net NN ferromagnetic interaction J_{net} evaluated for the 1D chain in the cuprates is about few Hundred K,[17] which corresponds to $J(\sim J_{net} + 4t^2/U) \sim 0.5t$, if we adopt the band calculation result of $t \sim 0.1$ eV for $Sr_{14}Cu_{14}O_{41}$,[15] and assume $U \sim O(10t)$. As mentioned above, $J \sim 0.5t$ is enough to suppress the spin gap for the cases investigated at half-filling, and might even produce ferromagnetism. Thus, the situation corresponding to the real materials is subtle, and the ground state may become weakly ferromagnetic depending on the details of the parameter values, which may also be consistent with the small Curie temperature of ~ 10 K observed experimentally.[18,20] The present results suggest that the weakly ferromagnetic behavior of the susceptiblity is not due to the interactions being extremely weak, but due to the 'cancellation effect' between t' and J.

On the other hand, the spin gap is observed for the 1D chain in $Sr_{14}Cu_{24}O_{41}$ with $\Delta_S \sim 140$K, which corresponds to $\sim 0.1t$ (assuming $t \sim 0.1$ eV) in the t-t'-U model. All our numerical results at quarter filling show that the spin gap is much smaller than $0.1t$, if any. Thus, we may conclude that the experimentally observed spin gap cannot be explained within t-t'-U or t-t'-U-J models. Then, some other ingredients, e.g., a coupling with the

lattice (which may be dimerized), should be necessary. Even in that case, there still remains a possibility that t' is playing an important role in opening the spin gap. Further investigation will be required to clarify this point.

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[25] In ref. 24, the ferromagnetic phase boundary $U_c(t')$ was determined for $n \leq 1$ at three points $t' = -0.2, -0.8$, and -2.0. We have more closely scanned the region $-0.8 \leq t' \leq -0.2$ at quarter-filling with DMRG, to find that, although $U_c(t' = -0.2) = 8$ and $U_c(t' = -0.8) = 20$ in agreement with ref. 24, $U_c(t')$ does not monotonically increases with $|t'|$ but U_c has in fact its minimum ($U_c = 4$) around $t' = -0.4$. Hence $U_c(t' = -0.55) \simeq 5$, so that the ground state at $t' = -0.55$ and $U = 8$ is fully polarized.

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FIGURES

FIG. 1. DMRG result for the spin gap, Δ_S, in the t-t'-U model plotted against the inverse system size $1/L$ for $t' = -0.8$, $U = 8$ with the band filling $n = 1$ or $n = 0.5$. Solid curves are least-square fits to second order polynomials in $1/L$.

FIG. 2. A plot similar to Fig. 1 for $t' = -0.55$, $U = 8$.

FIG. 3. A plot similar to Fig. 1 for for $t' = -2$, $U = 16$.

FIG. 4. A plot similar to Fig. 1 for the t-t'-U-J model for (a) $n = 1$, $t' = -0.8$, $U = 8$ and (b)$n = 0.5$, $t' = -2$, $U = 16$ with $J = 0.0$, $J = 0.5$ and 1.0

n=1.0

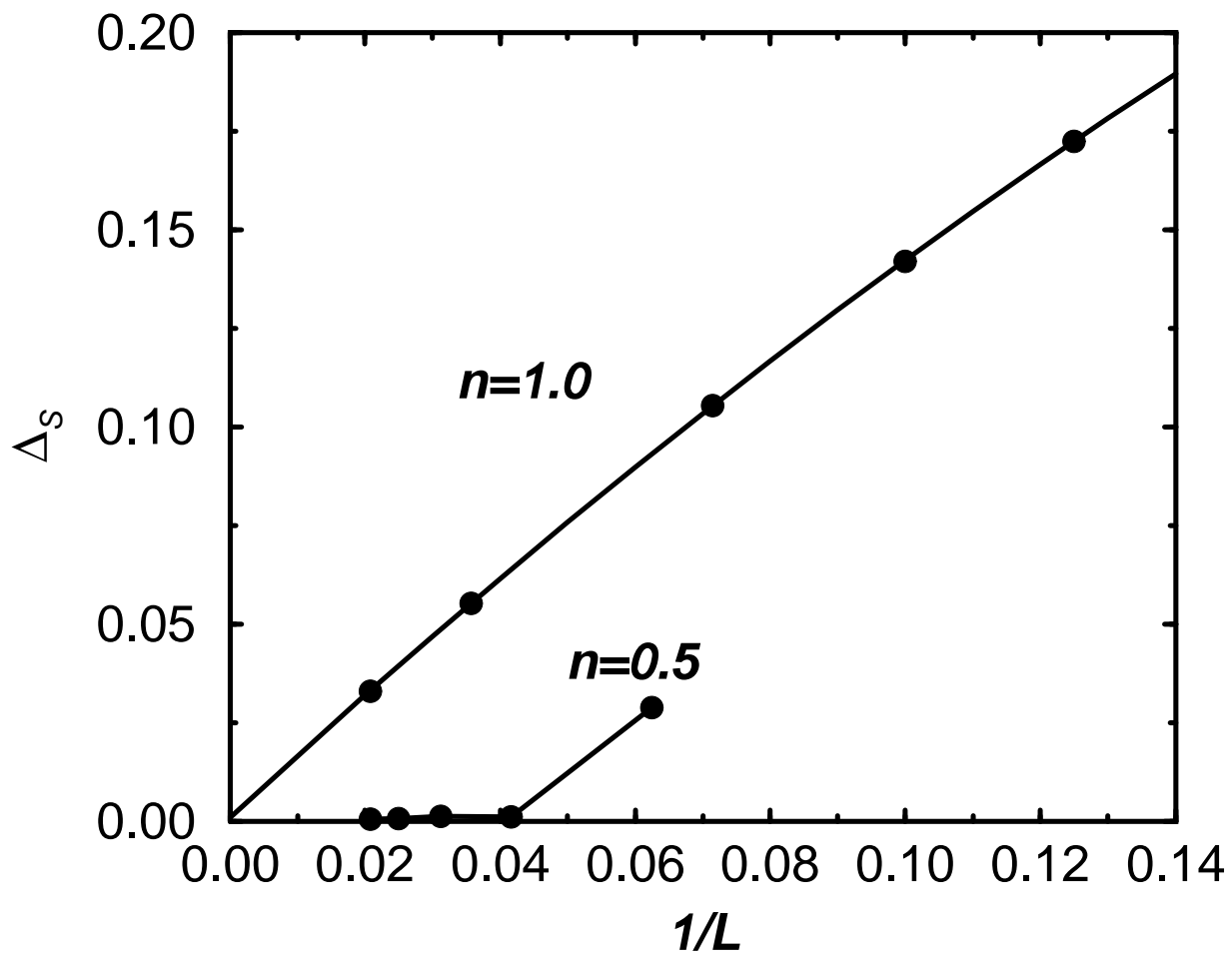n=0.5

Δ_S

1/L
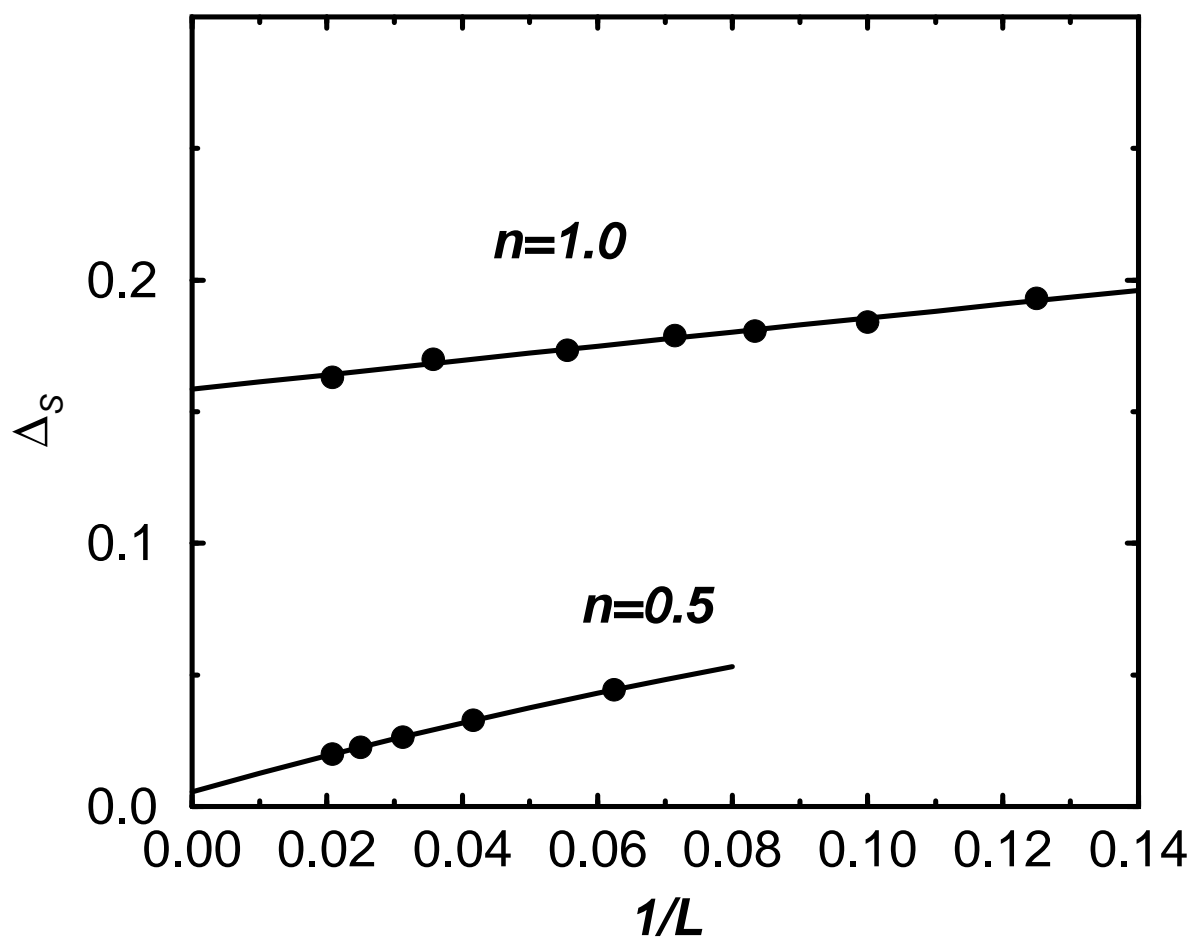
Fig.1

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Fig. 2

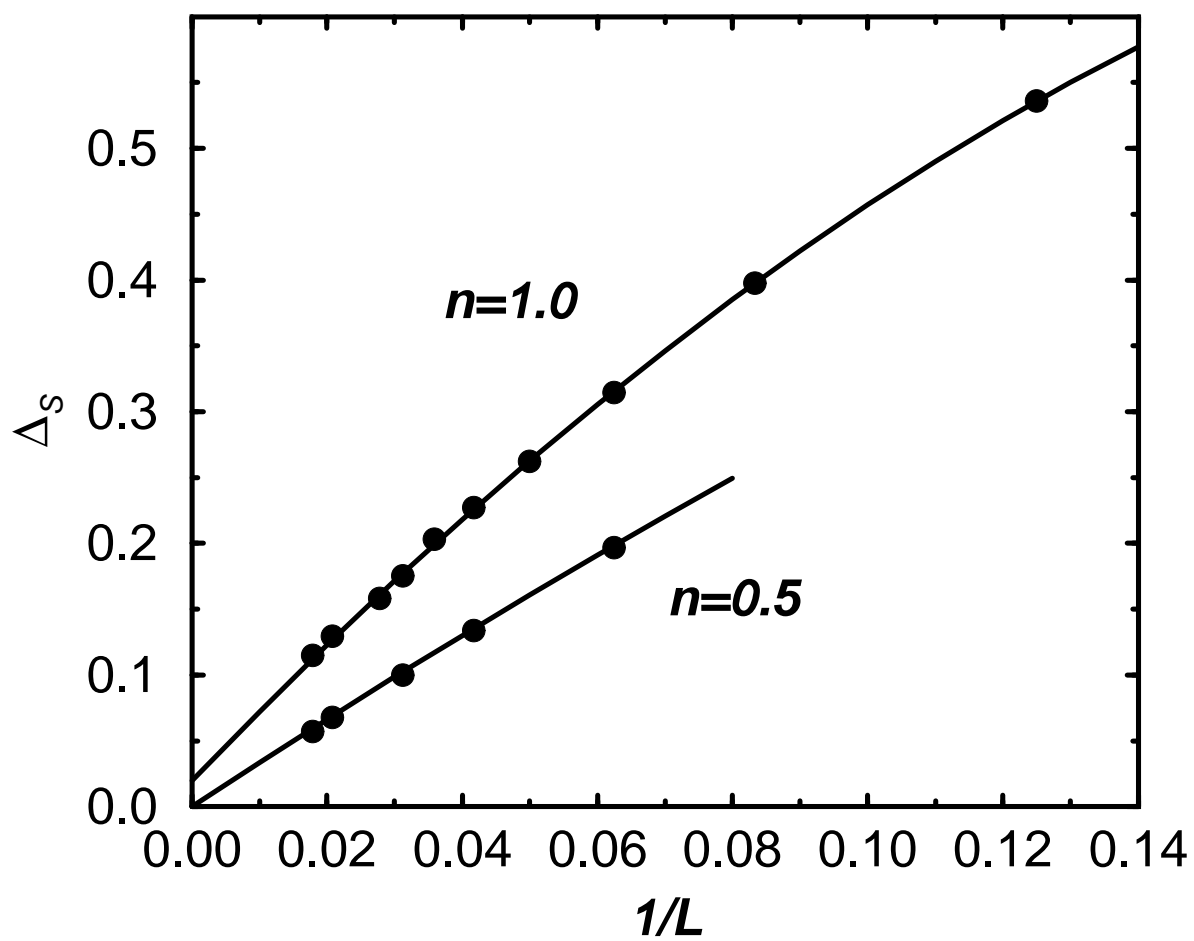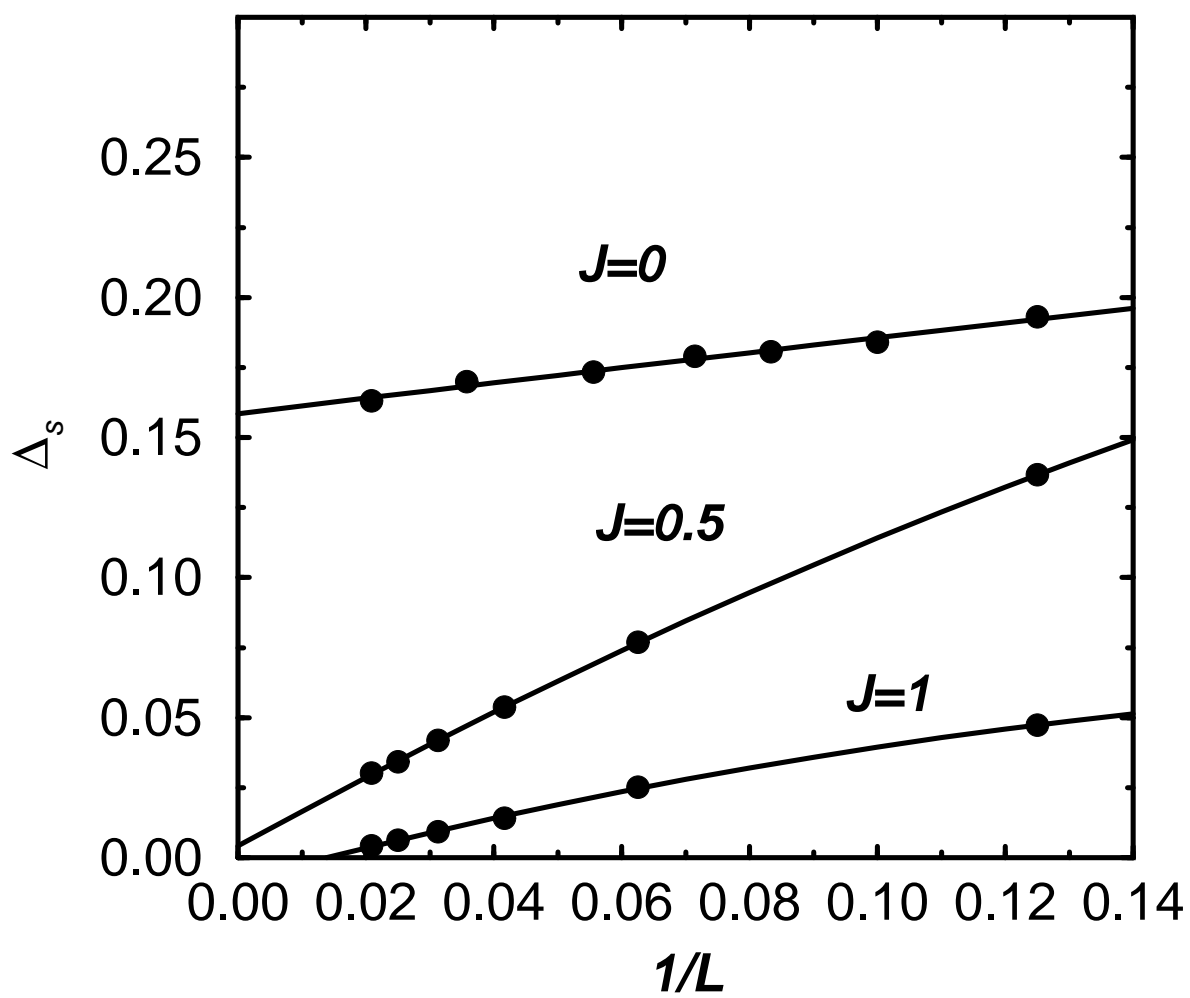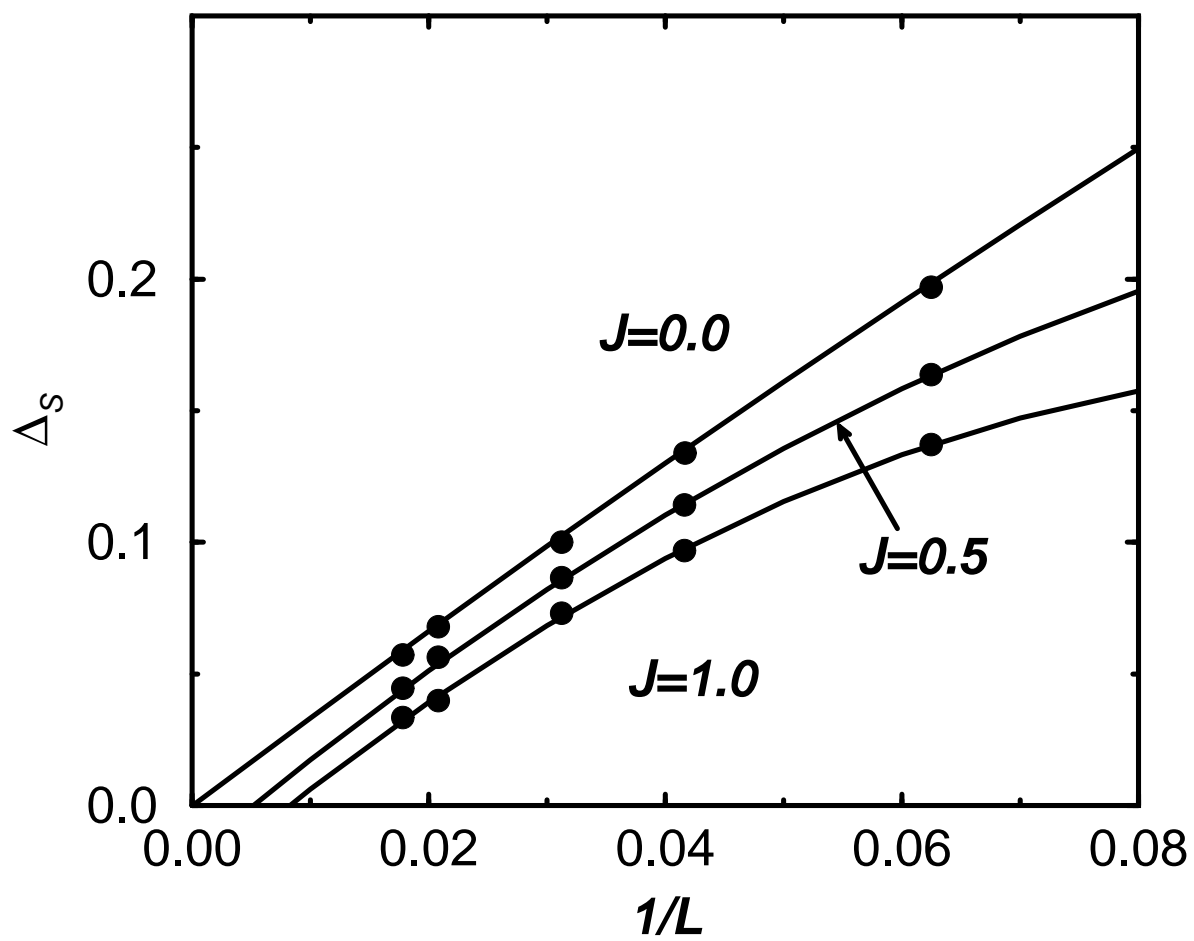Arita et al, Phys. Rev. B

Fig. 3

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Fig . 4a

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Fig. 4 b

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